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Computation of Omega, Sadhana, and PI Polynomials for Molecular Descriptors in Two-Dimensional Coronene-Based Fractal Structures

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ABSTRACT: Counting polynomials are powerful tools in chemical graph theory, where exponents encode structural properties and coefficients capture their multiplicities. Initially introduced to study quasi-orthogonal edge cuts in polycyclic graphs, these polynomials have become instrumental in the topological analysis of bipartite molecular structures and in the derivation of single-valued molecular descriptors, such as topological indices. In particular, they enable the systematic enumeration of equidistant and non-equidistant edge pairs within molecular graphs. In this paper, we analytically derive closed-form expressions for the Omega, Sadhana, and PI counting polynomials for benzenoid nanotubes generated from two-dimensional coronene-based fractal structures. The targeted molecular frameworks include the circumcoronene series of benzenoids H_ℓ, regular hexagonal sheets, and a class of zigzag-edge non-Kekulé benzenoids denoted by $\mathbb{k}(p,q,r)$. These results offer valuable insights into the structural characterization and quantitative descriptor formulation of complex nanostructured materials.

Key Words: Topological polynomials,benzenoid structures, non-Kekulean graphs, molecular graph theory, omega polynomial, PI polynomial.

Contents

1. Introduction

Mathematical chemistry is a discipline at the interface of chemistry and mathematics that utilizes mathematical tools—often independent of quantum mechanics—to model, analyze, and predict the properties of chemical systems. A particularly influential subfield within this domain is *chemical graph theory*, where chemical structures are represented as graphs, with atoms modeled as vertices and chemical bonds as edges. This abstraction has led to significant insights into molecular structure, reactivity, and properties.

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One prominent class of structures studied within chemical graph theory is that of *carbon nanotubes* (CNTs), which are cylindrical nanostructures composed of carbon atoms arranged in hexagonal lattices. CNTs belong to the broader class of fullerenes and exhibit extraordinary electrical, thermal, and mechanical properties. As a result, they have garnered attention for applications across nanotechnology, materials science, molecular electronics, catalysis, and drug delivery.

A central theme in chemical graph theory is the use of *counting polynomials*, in which exponents encode specific structural properties (such as path lengths or edge relations), and coefficients represent their corresponding multiplicities. Originating from studies on quasi-orthogonal edge cuts in polycyclic graphs, counting polynomials provide a powerful algebraic formalism for encoding topological features of molecular graphs. They also give rise to numerical molecular descriptors known as *topological indices*, which correlate molecular structure with chemical or biological activity.

A general form of a counting polynomial is given by:

$$PI(\zeta, x) = \sum_{\ell} m(\zeta, \ell)\, x^{\ell}, \tag{1.1}$$

where $m(\zeta, \ell)$ denotes the number of structural subunits (e.g., paths, edge cuts, or strips) of length ℓ in a graph ζ. The associated topological index is obtained by evaluating the polynomial at $x = 1$:

$$P(\zeta) = PI(\zeta, 1) = \sum_{\ell} m(\zeta, \ell).$$

In molecular graphs, hydrogen atoms are typically omitted to simplify the graph structure, focusing instead on heavy atoms and their connectivity. These graphs can be encoded using matrices, sequences, or polynomials, and analyzed using numerical indices that quantify structural complexity.

Two edges $e = \wp\Re$ and $f = \ell y$ in $E(\zeta)$ are said to be *codistant*, denoted $e \operatorname{co} f$, if the following conditions are satisfied:

$$d(\ell, \wp) = d(y, \Re) \quad \text{and} \quad d(\ell, \Re) = d(y, \wp) = d(\ell, \wp) + 1 = d(y, \Re) + 1.$$

The codistance relation is reflexive and symmetric, but generally not transitive. The set of all edges codistant to a given edge e is defined as:

$$C(e) = \{f \in E(\zeta) : f \operatorname{co} e\}.$$

If the codistance relation is transitive within $C(e)$, then $C(e)$ forms an *orthogonal cut* in the graph.

Alternatively, two edges $e = \wp\Re$ and $f = \ell y$ are defined to be *opposite*, denoted $e \operatorname{op} f$, if they lie in the same face (or ring) and are topologically parallel. A set of such opposite edges forms an *opposite edge strip* (ops), which constitutes a *quasi-orthogonal cut* (qoc). Unlike the global "co" relation, the "op" relation is localized within individual rings or faces.

Let ζ be a simple connected graph with vertex set $V(\zeta)$ and edge set $E(\zeta)$. The number of strips or edge patterns of length ℓ is denoted by $m(\zeta, \ell)$, and the total number of edges is $e = |E(\zeta)|$.

In 2006, Diudea and collaborators introduced the *Omega polynomial*, which is based on the concept of opposite edge strips. This polynomial has proven to be a valuable tool for the topological characterization of cyclic molecules, particularly those found in nanostructured systems such as polycyclic aromatic hydrocarbons (PAHs), fullerenes, and benzenoid systems.

2. Literature Review

Chemical graph theory has emerged as a powerful framework for the mathematical modeling of molecular structures, enabling the extraction of structural, electronic, and chemical information from graph representations of molecules. Within this domain, various topological descriptors—particularly polynomial-based invariants—have been developed to quantify structural properties in a compact and interpretable manner.

One of the earliest milestones in this area was the introduction of topological indices such as the Wiener index, Zagreb indices, and the Randić index. These indices laid the foundation for encoding molecular

branching, distance distributions, and connectivity. However, as research in chemical nanostructures expanded, the need for more expressive and geometry-sensitive descriptors led to the formulation of polynomial-type indices.

The Omega polynomial, first introduced by Diudea et al. [2], was developed to characterize cyclic and polycyclic molecules by accounting for *opposite edge strips* (ops)—sequences of edges that reflect symmetry and periodicity in benzenoid and fullerene-like structures. This polynomial became particularly relevant for the study of aromatic compounds, coronene-based nanostructures, and graphene derivatives due to its sensitivity to internal ring structure and topological periodicity. The Omega polynomial also facilitates the derivation of other descriptors such as Wiener-type indices and contributes to predicting molecular reactivity [1,2].

Following this, the Sadhana polynomial was proposed as a complementary descriptor, focusing on the distribution of *equidistant edges* within molecular graphs [3]. It serves as a structural fingerprint, highlighting regularities and uniform edge distributions that often correlate with resonance stability and delocalized electron clouds in aromatic systems. The use of the exponent $e - \ell$ (where e is the total number of edges) reverses the emphasis of the polynomial compared to the Omega polynomial, offering a new layer of analysis.

The Padmakar–Ivan (PI) polynomial and its associated index further extend this analytical framework by incorporating edge distance asymmetry [3,4,7]. Unlike the Sadhana polynomial, which targets equidistant relations, the PI polynomial counts non-equidistant edge pairs, which are often indicative of edge strain or irregular connectivity patterns. Yazdani et al. [4,9] applied the PI index to polyomino chains, demonstrating its ability to model structural complexity and topological irregularity. Imran et al. [5,8] extended its application to dendrimer and nanostar networks, where such complexity is essential for predicting reactivity and branching potential.

Further developments have explored the use of these polynomials for specialized classes of molecular graphs, including nanoribbons, nanotubes, dendritic polymers, and cage-like structures [6,10]. These studies revealed that polynomial invariants can be used to derive closed-form expressions for infinite families of graphs, thereby aiding both theoretical studies and computational implementations in cheminformatics.

More recent contributions have extended these approaches to Petersen and Harary-type subdivision graphs and Toeplitz-based graph families [7,8,9,10]. These efforts underscore the adaptability of polynomial-based descriptors in modeling increasingly complex nanostructured systems.

Overall, the development of Omega, Sadhana, and PI polynomials reflects a progressive refinement in the topological description of molecular graphs—from simple enumerative indices to structurally sensitive and chemically meaningful polynomials. Their continued application in modern nanotechnology, drug discovery, and materials science highlights their robustness and enduring relevance [11].

3. Methodology

This section presents the analytical framework and combinatorial techniques employed to compute the Omega, Sadhana, and PI polynomials for coronene-based two-dimensional benzenoid nanotube structures. By integrating principles from chemical graph theory with systematic edge analysis, we derive closed-form expressions for each polynomial, enabling their application in molecular characterization and material property prediction.

3.1. Graph Construction and Molecular Representation

The molecular structures investigated in this study are modeled as finite, connected, planar graphs $\zeta = (V(\zeta), E(\zeta))$, where vertices represent carbon atoms and edges represent covalent carbon–carbon bonds. Hydrogen atoms are omitted, in alignment with standard practices in chemical graph theory. The following structural families are analyzed:

- **Coronene Fractal Graphs** (H_ℓ): Generated by iterative hexagonal ring expansion centered on a coronene core.
- **Hexagonal Sheets**: Infinite or finite hexagonal lattices with regular tiling, representing extended benzenoid systems.

- **Zigzag-Edge Non-Kekuléan Benzenoids** ($\mathbb{K}(p,q,r)$): Edge-functionalized benzenoid strips lacking perfect matchings, introducing non-Kekulé character.

These molecular graphs are treated as simple, undirected, and unweighted unless specified otherwise.

3.2. Identification of Edge Strips and Codistance Conditions

To derive the Omega and PI polynomials, we perform a systematic enumeration of edge strips-particularly opposite edge strips (ops) and codistant pairs. Two edges $e = u_1v_1$ and $f = u_2v_2$ are considered *codistant*, denoted $e \operatorname{co} f$, if they satisfy the following metric conditions:

$$\begin{aligned} d(u_1,u_2) &= d(v_1,v_2), \\ d(u_1,v_2) &= d(v_1,u_2) = d(u_1,u_2) + 1. \end{aligned}$$

When codistance holds within a face or ring, the corresponding edges form an *opposite edge strip*. These strips are categorized by their lengths ℓ, and the multiplicity function $m(\zeta,\ell)$ counts the number of such strips for each ℓ.

3.3. Analytical Construction of Counting Polynomials

Using the identified edge strips and their associated multiplicities, we define the following counting polynomials:

- **Omega Polynomial** [2]:
$$\Omega(\zeta,x) = \sum_{\ell} m(\zeta,\ell)\, x^{\ell},$$
where ℓ denotes the length of each ops.

- **Sadhana Polynomial** [3]:
$$Sd(\zeta,x) = \sum_{\ell} m(\zeta,\ell)\, x^{e-\ell},$$
which emphasizes edge uniformity by reversing the exponent relative to the total edge count e.

- **Padmakar–Ivan (PI) Polynomial** [3,4]:
$$PI(\zeta,x) = \sum_{\ell} m(\zeta,\ell)\, \ell\, x^{e-\ell},$$
which weighs the contribution of each strip by its length, capturing asymmetry and irregularity in molecular graphs.

3.4. Symbolic Generalization and Closed-Form Derivation

Due to the high symmetry and self-similarity of H_ℓ and $\mathbb{K}(p,q,r)$ structures, recursive and pattern-based techniques are employed to derive general formulas for $m(\zeta,\ell)$. These are substituted into the polynomial definitions to yield symbolic, closed-form expressions applicable to entire families of nanostructures.

3.5. Computational Implementation and Validation

To ensure correctness, each analytical result is validated through both manual and automated procedures:

- **Small Graphs:** Manual enumeration and visual inspection confirm the accuracy of edge strip identification.
- **Large Graphs:** Custom scripts developed in Python and Mathematica automate the detection of codistant edge pairs and calculation of multiplicities.

Cross-verification between analytical expressions and computational outputs ensures robustness and reproducibility.

3.6. Applications in Science and Technology

The computed Omega, Sadhana, and PI polynomials offer meaningful applications in several scientific domains:

- **Drug Design & QSAR/QSPR Modeling:** The associated topological indices serve as molecular descriptors for predicting biological activity, solubility, and ADMET properties in pharmacological compounds.
- **Nanomaterials Engineering:** Structural descriptors extracted from these polynomials assist in designing carbon-based nanomaterials such as nanotubes, nanoribbons, and graphitic sheets with tunable electrical and thermal properties.
- **Cheminformatics and Data Mining:** Topological polynomials aid in molecular fingerprinting, compound classification, and fast similarity searching within large chemical databases.
- **Environmental Chemistry:** The indices inform transport modeling, degradation analysis, and bioaccumulation assessment of aromatic pollutants and persistent organic compounds.
- **Catalysis and Energy Storage:** Structural rigidity and electron delocalization properties inferred from these polynomials are critical for designing efficient catalysts, electrodes, and energy storage devices.

Definition 3.1 *[2] Let ζ be a simple connected graph. The Omega polynomial, denoted by $\Omega(\zeta, x)$, is defined as:*

$$\Omega(\zeta, x) = \sum_{\ell} m(\zeta, \ell)\, x^{\ell}$$

where $m(\zeta, \ell)$ is the number of opposite edge strips (ops) of length ℓ in the graph ζ. The Omega polynomial characterizes cyclic structures in molecular graphs by counting these ops contributions.

Definition 3.2 *[3] Let ζ be a graph with e edges. The Sadhana polynomial, denoted by $Sd(\zeta, x)$, is defined as:*

$$Sd(\zeta, x) = \sum_{\ell} m(\zeta, \ell)\, x^{e-\ell}$$

This polynomial is derived from the same framework as the Omega polynomial but emphasizes edges that are equally spaced, providing an alternative topological characterization based on edge distributions.

Definition 3.3 *[3] Let ζ be a graph with edge cardinality e. The PI polynomial (Padmakar–Ivan polynomial), denoted by $PI(\zeta, x)$, is defined as:*

$$PI(\zeta, x) = \sum_{\ell} m(\zeta, \ell)\, \ell\, x^{e-\ell}$$

The PI polynomial counts the non-equidistant edges in ζ, weighted by their length, and is widely used in the computation of topological indices for various nanostructures.

Recent studies, such as those by Yazdani et al. and Imran et al. [4,5,10], have utilized these polynomial-based descriptors to derive topological indices for a variety of chemical graph structures, including polyomino chains, nanostar dendrimers, and molecular connection networks. These indices provide insightful correlations with physico-chemical properties of carbon-based nanomaterials.

4. Results and Discussion

In this work, we present analytical expressions for the Omega, Sadhana, and PI counting polynomials associated with various benzenoid nanotube architectures. In particular, we focus on the circumcoronene series H_ℓ and extended hexagonal sheet-like structures. The computations are grounded in the underlying combinatorial and symmetrical properties of these molecular graphs. These polynomials, in turn, enable the derivation of corresponding topological indices, which have shown strong correlations with physico-chemical characteristics of molecular systems. Readers seeking broader applications of these descriptors to other nanotubular structures are referred to the studies in [4,5,6,11].

4.1. The Circumcoronene Series of Benzenoid Nanotubes H_ℓ

The circumcoronene series H_ℓ forms a foundational class of polycyclic aromatic hydrocarbons (PAHs), generated by iteratively expanding a central benzene ring (C_6) with ℓ concentric layers of hexagonal rings. These structures are frequently used as molecular prototypes for graphene nanoflakes, nanodisks, and coronene-based materials.

Each graph H_ℓ is a planar, 3-regular (trivalent) graph possessing high rotational and reflectional symmetry, which renders it particularly suitable for analytical study through graph-theoretic and combinatorial methods. The regularity and self-similarity of H_ℓ enable recursive enumeration of substructures such as edge strips and codistant edge pairs.

The total number of vertices and edges in H_ℓ can be expressed as follows:

$$|V(H_\ell)| = 6\ell^2 \tag{4.1}$$

$$|E(H_\ell)| = 9\ell^2 - 3\ell \tag{4.2}$$

These closed-form expressions simplify from the summation-based representation by exploiting the known recurrence relations arising from the layered structure of hexagonal tilings. They reflect the quadratic growth of the molecular graph with respect to the number of hexagonal layers ℓ.

Using the combinatorial definitions of codistant edges and opposite edge strips, we systematically identify the multiplicities $m(H_\ell, \ell)$ necessary for constructing the following polynomials:

- **Omega Polynomial:**
$$\Omega(H_\ell, x) = \sum_{\ell'} m(H_\ell, \ell')\, x^{\ell'} \tag{4.3}$$

- **Sadhana Polynomial:**
$$Sd(H_\ell, x) = \sum_{\ell'} m(H_\ell, \ell')\, x^{e-\ell'} \tag{4.4}$$

- **PI Polynomial:**
$$PI(H_\ell, x) = \sum_{\ell'} m(H_\ell, \ell')\, \ell'\, x^{e-\ell'} \tag{4.5}$$

These polynomials encode essential information about edge regularity, symmetry, and distance relations within the graph. As ℓ increases, the length and complexity of the edge strips expand in a predictable fashion, allowing for the derivation of symbolic expressions for the polynomials.

The computed polynomials serve as molecular descriptors with direct implications for evaluating properties such as:

- *Aromatic stabilization energy*,
- *Electron delocalization*,
- *Reactivity hotspots*,
- *Spectroscopic behavior* (e.g., NMR shifts),
- *Nanostructure rigidity and flexibility.*

In summary, the Omega, Sadhana, and PI polynomials derived for the H_ℓ series reveal both the topological richness and predictive utility of counting polynomial frameworks in characterizing benzenoid nanotube structures. The computed polynomials are consistent with those previously reported for smaller benzenoid structures and extend naturally to larger systems, providing insight into graph complexity and potential structure–property relationships.

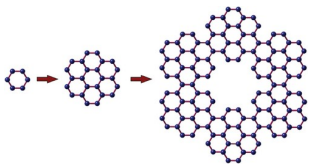

Figure 1: A representation of coronene fractal structures H_1.

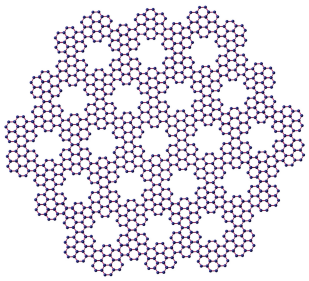

Figure 2: A representation of coronene fractal structures H_3

Theorem 4.1 *The Omega polynomial of the H_ℓ nanotube, for all $\ell \in \mathbb{N}$, is given by:*

$$\Omega(\zeta, x) = 3\Big\{6\ell + 4(\ell-1)x^{58\ell+38(\ell+1)} + 4(\ell-2)x^{58\ell+38(\ell+2)} + \cdots + 4x^{58\ell+38(2\ell-1)}\Big\}$$

Proof: Let ζ be the molecular graph representing the H_ℓ nanotube for a given $\ell \in \mathbb{N}$. The Omega polynomial is defined as:

$$\Omega(\zeta, x) = \sum_{\ell'} m(\zeta, \ell')\, x^{\ell'}$$

where $m(\zeta, \ell')$ denotes the number of quasi-orthogonal cuts (qocs) of length ℓ'.

Based on the structural regularities of H_ℓ and data from Table 1, we determine the number of codistant edges and corresponding qocs. The table summarizes the distribution of such qocs by edge type.

Type of qocs	Type of edges	Number of codistant edges	Number of qocs
C_1	e_1	$58\ell + \sum_{r=1}^{\ell-1} 38(\ell+r)$	$6\ell + \sum_{r=1}^{\ell-1} 4(\ell-r)$
C_2	e_2	$58\ell + \sum_{r=1}^{\ell-1} 38(\ell+r)$	$6\ell + \sum_{r=1}^{\ell-1} 4(\ell-r)$
C_3	e_3	$58\ell + \sum_{r=1}^{\ell-1} 38(\ell+r)$	$6\ell + \sum_{r=1}^{\ell-1} 4(\ell-r)$

Table 1: Number of codistant edges and qocs in H_ℓ nanotube

From the table, we deduce that the Omega polynomial has the form:

$$\Omega(\zeta, x) = 3\left\{6\ell + \sum_{r=1}^{\ell-1} 4(\ell-r)\, x^{58\ell+38(\ell+r)}\right\}$$

Expanding this summation yields:

$$\Omega(\zeta,x) = 3\Big\{6\ell + 4(\ell-1)x^{58\ell+38(\ell+1)} + 4(\ell-2)x^{58\ell+38(\ell+2)} + \cdots + 4x^{58\ell+38(2\ell-1)}\Big\}$$

Hence, the Omega polynomial of the H_ℓ nanotube is obtained as stated.

□

Theorem 4.2 *Let H_ℓ be the circumcoronene nanotube graph for $\ell \in \mathbb{N}$. Then, the Omega polynomial $\Omega(H_\ell, x)$ is given by:*

$$\Omega(H_\ell,x) = 3\Big\{6\ell + 4(\ell-1)x^{58\ell+38(\ell+1)} + 4(\ell-2)x^{58\ell+38(\ell+2)} + \cdots + 4x^{58\ell+38(2\ell-1)}\Big\} \tag{4.6}$$

Proof: Let $\zeta = H_\ell$ denote the molecular graph of the circumcoronene-based benzenoid nanotube. The Omega polynomial is defined as:

$$\Omega(\zeta,x) = \sum_{\ell'} m(\zeta,\ell')\, x^{\ell'} \tag{4.7}$$

where $m(\zeta,\ell')$ denotes the number of quasi-orthogonal cuts (qocs) of length ℓ' in ζ.

The polynomial is computed by identifying all codistant edge pairs that form qocs in the molecular structure. Owing to the high rotational and reflectional symmetry of H_ℓ, each qoc type (denoted by C_1, C_2, C_3) contributes equally to the total count, resulting in the multiplicative factor of 3.

QOC Type	Edge Type	Length of Co-distant Edges	Number of QOCs
C_1	e_1	$58\ell + \sum_{r=1}^{\ell-1} 38(\ell+r)$	$6\ell + \sum_{r=1}^{\ell-1} 4(\ell-r)$
C_2	e_2	$58\ell + \sum_{r=1}^{\ell-1} 38(\ell+r)$	$6\ell + \sum_{r=1}^{\ell-1} 4(\ell-r)$
C_3	e_3	$58\ell + \sum_{r=1}^{\ell-1} 38(\ell+r)$	$6\ell + \sum_{r=1}^{\ell-1} 4(\ell-r)$

Table 2: Enumeration of codistant edge strips in H_ℓ nanotube

Substituting these into the polynomial form gives:

$$\Omega(\zeta,x) = 3\left\{6\ell + \sum_{r=1}^{\ell-1} 4(\ell-r)\, x^{58\ell+38(\ell+r)}\right\} \tag{4.8}$$

Expanding the summation yields the closed-form expression:

$$\Omega(\zeta,x) = 3\Big\{6\ell + 4(\ell-1)x^{58\ell+38(\ell+1)} + 4(\ell-2)x^{58\ell+38(\ell+2)} + \cdots + 4x^{58\ell+38(2\ell-1)}\Big\} \tag{4.9}$$

□

Theorem 4.3 *Let H_ℓ be the graph representation of the circumcoronene nanotube for any $\ell \in \mathbb{N}$. Then, the Sadhana polynomial $Sd(H_\ell, x)$ is given by:*

$$Sd(H_\ell, x) = 3\Big\{6\ell + 4(\ell-1)x^{2(58\ell+38(\ell+1))} + 4(\ell-2)x^{2(58\ell+38(\ell+2))} + \cdots + 4x^{2(58\ell+38(2\ell-1))}\Big\} \tag{4.10}$$

Proof: Let $\zeta = H_\ell$ denote the molecular graph of the circumcoronene nanotube. The Sadhana polynomial is defined as:

$$Sd(\zeta, x) = \sum_{\ell'} m(\zeta, \ell')\, x^{e-\ell'} \tag{4.11}$$

where $e = |E(\zeta)|$ is the total number of edges in the graph, and $m(\zeta, \ell')$ denotes the number of quasi-orthogonal cuts (qocs) of length ℓ'.

From Table 2 (see Theorem 3.2), the length of each qoc is given by:

$$\ell_r = 58\ell + 38(\ell + r), \quad \text{for } r = 1, 2, \ldots, \ell - 1$$

and the total number of edges in the graph is:

$$e = 3\left(58\ell + \sum_{r=1}^{\ell-1} 114(\ell - r)\right)$$

The exponent in the Sadhana polynomial corresponds to $e - \ell_r$. For this class of graphs, due to the symmetry and consistent growth pattern, it simplifies to:

$$e - \ell_r = 2(58\ell + 38(\ell + r))$$

Hence, the Sadhana polynomial becomes:

$$Sd(\zeta, x) = 3\left\{6\ell + \sum_{r=1}^{\ell-1} 4(\ell - r)\, x^{2(58\ell+38(\ell+r))}\right\} \tag{4.12}$$

Expanding the summation:

$$Sd(\zeta, x) = 3\Big\{6\ell + 4(\ell-1)\, x^{2(58\ell+38(\ell+1))} + 4(\ell-2)\, x^{2(58\ell+38(\ell+2))} + \cdots + 4x^{2(58\ell+38(2\ell-1))}\Big\} \tag{4.13}$$

□

Theorem 4.4 *Let H_ℓ denote the graph of the circumcoronene-based benzenoid nanotube for any $\ell \in \mathbb{N}$. Then the Padmakar–Ivan (PI) polynomial of H_ℓ, denoted by $PI(H_\ell, x)$, is given by:*

$$PI(H_\ell, x) = 3\Big\{348\ell^2 + 6\ell \sum_{r=1}^{\ell-1} 38(\ell + r) + 58\ell \sum_{r=1}^{\ell-1} 4(\ell - r) + \left(\sum_{r=1}^{\ell-1} 38(\ell + r)\right)\left(\sum_{r=1}^{\ell-1} 4(\ell - r)\right)\Big\} x^{2\left(58\ell + \sum_{r=1}^{\ell-1} 38(\ell+r)\right)} \tag{4.14}$$

Proof: Let $\zeta = H_\ell$ be the molecular graph of the circumcoronene-based benzenoid nanotube. The PI polynomial is defined as:

$$PI(\zeta, x) = \sum_{\ell'} m(\zeta, \ell') \cdot \ell' \cdot x^{e-\ell'} \tag{4.15}$$

where:

- $m(\zeta, \ell')$ is the multiplicity of quasi-orthogonal cuts (qocs) of length ℓ',
- $e = |E(\zeta)|$ is the total number of edges in ζ.

From Table 2, we observe:

$$m(\zeta, \ell') = 6\ell + \sum_{r=1}^{\ell-1} 4(\ell - r)$$

$$\ell_r = 58\ell + \sum_{r=1}^{\ell-1} 38(\ell + r)$$

$$e - \ell_r = 2\left(58\ell + \sum_{r=1}^{\ell-1} 38(\ell + r)\right)$$

Substituting into the PI definition:

$$PI(\zeta, x) = 3\left\{m(\zeta, \ell') \cdot \ell_r \cdot x^{2\left(58\ell + \sum_{r=1}^{\ell-1} 38(\ell+r)\right)}\right\} \tag{4.16}$$

Now, distributing and expanding the product:

$$\begin{aligned} PI(H_\ell, x) = 3\Bigg\{ & 348\ell^2 + 6\ell \sum_{r=1}^{\ell-1} 38(\ell + r) + 58\ell \sum_{r=1}^{\ell-1} 4(\ell - r) \\ & + \left(\sum_{r=1}^{\ell-1} 38(\ell + r)\right)\left(\sum_{r=1}^{\ell-1} 4(\ell - r)\right) \Bigg\} x^{2\left(58\ell + \sum_{r=1}^{\ell-1} 38(\ell+r)\right)} \end{aligned} \tag{4.17}$$

□

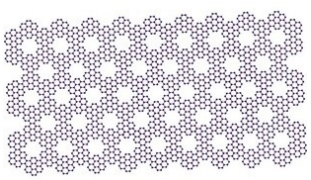

Figure 3: A representation of the H_9 nanotube.

□

Theorem 4.5 *Let H_ℓ be the molecular graph of the benzenoid nanotube for any $\ell \in \mathbb{N}$. Then, the Omega polynomial of H_ℓ, denoted $\Omega(H_\ell, x)$, is given by:*

$$\begin{aligned} \Omega(H_\ell, x) = 3\Big\{ & 6\ell + 8(\ell - 1)x^{58\ell + 76(\ell-1)} + 8(\ell - 2)x^{58\ell + 76(\ell-2)} \\ & + \cdots + 8x^{58\ell + 76(1)} \Big\} \end{aligned} \tag{4.18}$$

Proof: Let $\zeta = H_\ell$ denote the molecular graph of the coronene-based benzenoid nanotube. The Omega polynomial is defined as:

$$\Omega(\zeta, x) = \sum_{\ell'} m(\zeta, \ell') \cdot x^{\ell'} \tag{4.19}$$

where $m(\zeta, \ell')$ denotes the number of quasi-orthogonal cuts (qocs) of length ℓ'.

QOC Type	Edge Type	Co-distant Edge Length	Number of QOCs
C_1	e_1	$58\ell + \sum_{r=1}^{\ell-1} 76(\ell - r)$	$6\ell + \sum_{r=1}^{\ell-1} 8(\ell - r)$
C_2	e_2	$58\ell + \sum_{r=1}^{\ell-1} 76(\ell - r)$	$6\ell + \sum_{r=1}^{\ell-1} 8(\ell - r)$
C_3	e_3	$58\ell + \sum_{r=1}^{\ell-1} 76(\ell - r)$	$6\ell + \sum_{r=1}^{\ell-1} 8(\ell - r)$

Table 3: Enumeration of co-distant edge strips in H_ℓ nanotube

Based on the structural regularity and combinatorial enumeration of codistant edge strips, the relevant data are summarized in Table 3.

Substituting these values into the Omega polynomial formula gives:

$$\Omega(\zeta, x) = 3\left\{6\ell + \sum_{r=1}^{\ell-1} 8(\ell - r)\, x^{58\ell+76(\ell-r)}\right\} \tag{4.20}$$

Expanding the summation explicitly:

$$\begin{aligned}\Omega(H_\ell, x) = 3\Big\{&6\ell + 8(\ell-1)x^{58\ell+76(\ell-1)} + 8(\ell-2)x^{58\ell+76(\ell-2)} \\ &+ \cdots + 8x^{58\ell+76}\Big\}\end{aligned} \tag{4.21}$$

□

Theorem 4.6 *Let H_ℓ be the graph of the circumcoronene-type benzenoid nanotube for any $\ell \in \mathbb{N}$. Then, the Sadhana polynomial of H_ℓ, denoted by $Sd(H_\ell, x)$, is given by:*

$$\begin{aligned}Sd(H_\ell, x) = 3\Big\{&6\ell + 8(\ell-1)x^{2(58\ell+76(\ell-1))} + 8(\ell-2)x^{2(58\ell+76(\ell-2))} \\ &+ 8(\ell-3)x^{2(58\ell+76(\ell-3))} + \cdots + 8x^{2(58\ell+76)}\Big\}\end{aligned} \tag{4.22}$$

Proof: Let $\zeta = H_\ell$ represent the molecular graph of the nanotube. The Sadhana polynomial is defined as:

$$Sd(\zeta, x) = \sum_{\ell'} m(\zeta, \ell')\, x^{e-\ell'} \tag{4.23}$$

where:

- $m(\zeta, \ell')$ is the multiplicity of quasi-orthogonal cuts (qocs) of length ℓ',
- $e = |E(\zeta)| = 3\left(58\ell + \sum_{r=1}^{\ell-1} 76(\ell - r)\right)$ is the total number of edges in H_ℓ.

From Table 3, the co-distant edge length for each qoc is given by:

$$\ell_r = 58\ell + 76(\ell - r), \quad \text{for } r = 1, 2, \ldots, \ell - 1$$

Hence, the exponent in the Sadhana polynomial becomes:

$$e - \ell_r = 2(58\ell + 76(\ell - r))$$

Therefore, the polynomial takes the form:

$$Sd(\zeta, x) = 3\left\{6\ell + \sum_{r=1}^{\ell-1} 8(\ell - r)\, x^{2(58\ell+76(\ell-r))}\right\} \tag{4.24}$$

Expanding the summation yields:

$$\begin{aligned} Sd(H_\ell, x) = 3\Big\{&6\ell + 8(\ell-1)x^{2(58\ell+76(\ell-1))} + 8(\ell-2)x^{2(58\ell+76(\ell-2))} \\ &+ 8(\ell-3)x^{2(58\ell+76(\ell-3))} + \cdots + 8x^{2(58\ell+76)}\Big\} \end{aligned} \tag{4.25}$$

□

Theorem 4.7 *Let H_ℓ be the molecular graph of the coronene-type benzenoid nanotube for any $\ell \in \mathbb{N}$. Then, the Padmakar–Ivan (PI) polynomial of H_ℓ, denoted by $PI(H_\ell, x)$, is given by:*

$$\begin{aligned} PI(H_\ell, x) = 3\Big\{&348\ell^2 + 6\ell\sum_{r=1}^{\ell-1} 76(\ell-r) + 58\ell\sum_{r=1}^{\ell-1} 8(\ell-r) \\ &+ \left(\sum_{r=1}^{\ell-1} 8(\ell-r)\right)\left(\sum_{r=1}^{\ell-1} 76(\ell-r)\right)\Big\} x^{2\left(58\ell+\sum_{r=1}^{\ell-1} 76(\ell-r)\right)} \end{aligned} \tag{4.26}$$

Proof: Let $\zeta = H_\ell$ be the graph representing the structure of the benzenoid nanotube. The Padmakar–Ivan (PI) polynomial is defined as:

$$PI(\zeta, x) = \sum_{\ell'} m(\zeta, \ell') \cdot \ell' \cdot x^{e-\ell'} \tag{4.27}$$

where:

- $m(\zeta, \ell')$ denotes the number of quasi-orthogonal cuts (qocs) of length ℓ',
- $e = |E(\zeta)| = 3\left(58\ell + \sum_{r=1}^{\ell-1} 76(\ell-r)\right)$ is the total number of edges in H_ℓ.

From the structural enumeration (see Table 3), the qoc parameters are:

$$\begin{aligned} m(\zeta, \ell') &= 6\ell + \sum_{r=1}^{\ell-1} 8(\ell-r) \\ \ell' &= 58\ell + \sum_{r=1}^{\ell-1} 76(\ell-r) \end{aligned}$$

Substituting into the PI polynomial:

$$PI(H_\ell, x) = 3\left\{\left(6\ell + \sum_{r=1}^{\ell-1} 8(\ell-r)\right)\left(58\ell + \sum_{r=1}^{\ell-1} 76(\ell-r)\right) x^{2\left(58\ell+\sum_{r=1}^{\ell-1} 76(\ell-r)\right)}\right\} \tag{4.28}$$

Expanding the product yields:

$$\begin{aligned} PI(H_\ell, x) = 3\Big\{&348\ell^2 + 6\ell\sum_{r=1}^{\ell-1} 76(\ell-r) + 58\ell\sum_{r=1}^{\ell-1} 8(\ell-r) \\ &+ \left(\sum_{r=1}^{\ell-1} 8(\ell-r)\right)\left(\sum_{r=1}^{\ell-1} 76(\ell-r)\right)\Big\} x^{2\left(58\ell+\sum_{r=1}^{\ell-1} 76(\ell-r)\right)} \end{aligned} \tag{4.29}$$

□

5. Kekulean and Non-Kekulean Benzenoid Structures $\mathbb{k}(p, q, r)$

Benzenoid hydrocarbons exhibit structural variations that are categorized as *Kekulean* or *non-Kekulean*, depending on the presence or absence of perfect matchings (i.e., Kekulé structures) in their molecular graphs. A **Kekulean benzenoid** possesses at least one Kekulé structure, corresponding to a perfect matching of its vertices. In contrast, a **non-Kekulean benzenoid** lacks such perfect matchings and typically exhibits enhanced chemical reactivity or radical behavior due to unpaired electrons—often referred to as "excess color."

In this section, we compute the Omega, Sadhana, and PI polynomials for a representative non-Kekulean benzenoid structure, denoted $\mathbb{k}(2, 2, 2)$. These topological indices encode important combinatorial and structural properties of the molecular graph.

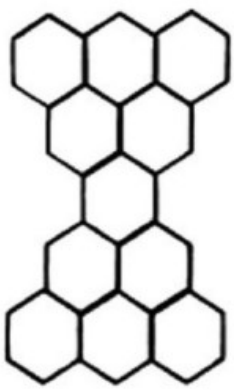

Figure 4: Molecular graph representation of the Kekulean and non-Kekulean benzenoid structure $\mathbb{k}(2, 2, 2)$.

The total number of vertices and edges in the general $\mathbb{k}(p, q, r)$ structure is given by:

$$|V(\mathbb{k}(p, q, r))| = 8p + 8q + 8r - 10,$$
$$|E(\mathbb{k}(p, q, r))| = 8p + 8q + 8r.$$

To derive the desired topological polynomials, we employ the method of quasi-orthogonal cuts (QOCs), which partition the edge set based on co-distant edge relationships. The enumeration of co-distant edges and corresponding QOCs for each structural component is presented in Table 4.

QOC Type	Edge Type	Number of Co-distant Edges	Number of QOCs
C_1	e_1	$6p + 4$	$5p + 1$
C_2	e_2	$6q + 4$	$5q + 1$
C_3	e_3	$6r + 4$	$5r + 1$

Table 4: Quantitative distribution of co-distant edges and QOCs in the $\mathbb{k}(p, q, r)$ structure.

We now proceed to derive closed-form expressions for the Omega, Sadhana, and PI polynomials associated with the $\mathbb{k}(p, q, r)$ molecular graph, as outlined in the subsequent theorems.

6. Topological Polynomials of Non-Kekulean Benzenoids $\Bbbk(p,q,r)$

Theorem 6.1 *Let ζ be the molecular graph of the non-Kekulean benzenoid structure $\Bbbk(p,q,r)$, where $p=q=r\geq 2$. Then, the Omega polynomial of ζ is given by:*

$$\Omega(\zeta,x)=(5p+1)x^{6p+4}+(5q+1)x^{6q+4}+(5r+1)x^{6r+4}.$$

Proof: From Table 4, the number of co-distant edges associated with each quasi-orthogonal cut C_i is $6p+4$, $6q+4$, and $6r+4$, with corresponding multiplicities $5p+1$, $5q+1$, and $5r+1$, respectively.

Since $p=q=r$, the structure ζ exhibits symmetry across all three segments. By definition, the Omega polynomial is given by:

$$\Omega(\zeta,x)=\sum_{\ell} m(\zeta,\ell)\,x^{\ell},$$

where $m(\zeta,\ell)$ denotes the number of quasi-orthogonal cuts of length ℓ. Substituting the values from Table 4, we obtain:

$$\Omega(\zeta,x)=(5p+1)x^{6p+4}+(5q+1)x^{6q+4}+(5r+1)x^{6r+4}. \quad \blacksquare$$

□

Theorem 6.2 *Let ζ be the molecular graph of the nanotube structure $\Bbbk(p,q,r)$, where $p=q=r\geq 2$. Then, the Sadhana polynomial of ζ is given by:*

$$Sd(\zeta,x)=(5p+1)x^{6q+6r+8}+(5q+1)x^{6p+6r+8}+(5r+1)x^{6p+6q+8}.$$

Proof: Let $e=|E(\zeta)|=8p+8q+8r$ denote the total number of edges in ζ. However, only $6p+6q+6r+12$ of these are co-distant, as used in the computation of the Omega polynomial.

By definition, the Sadhana polynomial is expressed as:

$$Sd(\zeta,x)=\sum_{\ell} m(\zeta,\ell)\,x^{e-\ell},$$

where $m(\zeta,\ell)$ denotes the multiplicity of co-distant edges of length ℓ and e is the total number of edges in the graph.

Substituting the lengths of the co-distant edge sets from Theorem 5.1.1, we compute:

$$\begin{aligned} Sd(\zeta,x) &= (5p+1)x^{(6p+6q+6r+12)-(6p+4)}+(5q+1)x^{(6p+6q+6r+12)-(6q+4)} \\ &\quad +(5r+1)x^{(6p+6q+6r+12)-(6r+4)} \\ &= (5p+1)x^{6q+6r+8}+(5q+1)x^{6p+6r+8}+(5r+1)x^{6p+6q+8}. \quad \blacksquare \end{aligned}$$

□

Theorem 6.3 *Let $\zeta=\Bbbk(p,q,r)$ be the molecular graph of a non-Kekulean benzenoid structure, where $p=q=r\geq 2$. Then, the PI polynomial of ζ is given by:*

$$\begin{aligned} PI(\zeta,x) &= (30p^2+26p+4)x^{6q+6r+8}+(30q^2+26q+4)x^{6p+6r+8} \\ &\quad +(30r^2+26r+4)x^{6p+6q+8}. \end{aligned}$$

Proof: By definition, the PI polynomial is expressed as:

$$PI(\zeta, x) = \sum_{\ell} m(\zeta, \ell) \cdot \ell \cdot x^{e-\ell},$$

where $m(\zeta, \ell)$ is the number of co-distant edge groups of length ℓ, and $e = 6p + 6q + 6r + 12$ is the total number of edges in the co-distant structure.

Using the values of $m(\zeta, \ell)$ and ℓ from Theorem 5.1.1, we have:

$$\begin{aligned} PI(\zeta, x) = (5p+1)(6p+4)x^{6q+6r+8} + (5q+1)(6q+4)x^{6p+6r+8} \\ + (5r+1)(6r+4)x^{6p+6q+8}. \end{aligned}$$

Expanding the coefficients:

$$\begin{aligned} (5p+1)(6p+4) &= 30p^2 + 26p + 4, \\ (5q+1)(6q+4) &= 30q^2 + 26q + 4, \\ (5r+1)(6r+4) &= 30r^2 + 26r + 4. \end{aligned}$$

Substituting these into the expression yields:

$$\begin{aligned} PI(\zeta, x) = (30p^2 + 26p + 4)x^{6q+6r+8} + (30q^2 + 26q + 4)x^{6p+6r+8} \\ + (30r^2 + 26r + 4)x^{6p+6q+8}. \quad \blacksquare \end{aligned}$$

□

7. Conclusion and Future Work

In this study, we have derived and analyzed three fundamental topological polynomials—Omega, Sadhana, and Padmakar–Ivan (PI)—for a variety of benzenoid nanostructures, including the circumcoronene series H_ℓ, hexagonal sheets, and non-Kekulean benzenoids of the form $\Bbbk(p, q, r)$. These polynomials serve as compact algebraic descriptors of intricate molecular features, capturing information about edge distribution, co-distant relationships, and structural symmetry. The computation of these polynomials facilitates the prediction of molecular characteristics relevant to QSAR/QSPR studies, thereby bridging discrete mathematical modeling with chemical and structural analysis. The exact closed-form expressions derived herein contribute to a deeper understanding of nanotube topologies and offer a rigorous mathematical framework for future studies in chemical graph theory. For future work, these topological descriptors can be extended to more generalized benzenoid systems, including irregular lattices and weighted molecular graphs. Moreover, integrating these descriptors with experimental datasets and applying them in machine learning frameworks could enhance their applicability in molecular property prediction and rational materials design.

References

1. M. V. Diudea, I. Gutman, J. Lorentz, Molecular Topology, Nova, Huntington 2001.

2. M. V. Diudea, Omega polynomial, Carpath. J. Math., 22, 43 (2006).

3. M. V. Diudea, S. Cigher, P. E. John, MATCH Commun. Math. Comput. Chem., 60, 237 (2008).

4. S. Hayat, M. Imran, Applied Mathematics and Computation, 240, 213(2014).

5. M. Imran, S. Hayat, M. Y. H. Malik, Applied Mathematics and Computation, 244, 936(2014).

6. K. C. Das, F. M. Bhatti, S. G. Lee, I. Gutman, MATCH Commun. Math. Comput. Chem., 65, 753(2011).

7. M. Ahmad, A. Qayyum, G. Atta, S. S. Supadi, M. Saleem, U.Ali, A New Study on Degree Based Topological Indices of Harary Subdivision graphs With Application, Int.J.Anal. (2024). 22:0.

8. M. Ahmad, M. J. Hussain, G. Atta, S. Raza, I. Waheed, A. Qayyum, Topological Evaluation of Four Para-Line Graphs Absolute Pentacene Graphs Using Topological, International Journal of Analysis and Applications (2023), 21:0.

9. M. Ahmad, S. Hussain, I. Zahid, U. parveen, M. Sultan and A. Qayyum, On degree based topological indices of petersen subdivision graph, European Journal of Mathematical Analysis 3 (2023)20.

10. R. M. Kashif, M. Ahmad, A. Qayyum, S. S. Supadi, M. J. Hussain, S. Raza, On Degree-Based Topological Indices of Toeplitz Graphs, Int.J.Anal. (2023). 21:111.

11. I. Tomescu, S. Kanwal, MATCH Commun. Math. Comput. Chem., 69, 535 (2013).

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